

Appendix C Modeling

C-1. Available Analytical and Numerical Models

Numerous analytical and digital models have been written to simulate pressure distributions, airflow, vapor transport, and extraction. In the past, many of these models were written for a specific purpose (e.g. a doctoral dissertation) and were not generally “maintained” as programs which could be easily obtained and used by design team members. Either that or many of the models were extremely complex and could only be used on a computer workstation or mainframe and consequently are not available to the typical engineer. However, advances in computing technology and software applications have enabled the development of several vadose zone multiphase models that incorporate complex mathematical solutions in a user-friendly program. Most of the well-recognized models are widely available and supported by various companies that promote environmental software. Table C-1 summarizes these soil vapor flow, contaminant transport, and extraction models, which were compiled primarily from conducting internet web searches and by including models currently being used in the field of vapor transport modeling. Each of the models presented can be run on PC system.

C-2. Pressure Distribution/Airflow

Pressure distribution/airflow models are analogous to groundwater flow models. They are constructed in a similar fashion, and they provide similar output. The one significant difference between the two types of models is that soil vapors are compressible gases for which densities, viscosities, and gas constants can vary depending on chemical composition, temperature, and pressure. Typical input parameters for pressure distribution/airflow models are as follows:

- Air permeability of soils (L^2).
- Flow rates from extraction points or to injection points (L^3/T).
- Air-filled soil porosity.
- Thickness of the vadose zone (L).
- Dynamic viscosity of vapor ($M/L-T$).
- Vapor temperature (degrees).
- Pressure boundary conditions ($M/L-T^2$).
- Output from pressure distribution/airflow models can include:
- Vapor pressure distributions ($M/L-T^2$).

- Flow rates from constant pressure nodes (L^3/T).
- Vapor velocities (L/T).
- Vapor “particle” pathlines.

a. The models listed in Table C-1 can all be used for these simulations. Those models, which are identified in Table C-1 as having an “easy” use, can typically be used by a project engineer with a strong background in fluids and soil science or geotechnical engineering. Project engineers who have experience using groundwater flow models typically have little difficulty using the simpler pressure distribution/airflow models. However, the input parameters and output from these models are less intuitively understood than those from groundwater flow models. Thus, novice modelers should always ensure that their work receives peer review from more experienced practitioners.

b. In many instances the pressure gradients imposed by SVE/BV systems are not large enough to cause significant density differences in soil vapors. In these instances, many engineers simply use existing groundwater models (with corrections for air permeabilities and air heads) to simulate soil vapor systems. Massmann (1989) provides an excellent description of the technique including detailed instructions and an analysis of limitations.

C-3. Coupled Fluid Flow and Contaminant Transport Models

Coupled fluid flow and contaminant transport models include airflow/contaminant transport models and multiphase flow/contaminant transport models. Both types involve two steps: solution of fluid flow equations to obtain fluid velocities, and solution of advection-dispersion equations to obtain contaminant concentrations. Most models including an airflow component involve solution by finite-difference or finite-element methods. These methods involve discretization of the model domain into nodes or cells.

a. For airflow and contaminant transport models, the pressure distribution is calculated by solution of the partial differential equation for airflow. Flow velocity is calculated using the pressure distribution in conjunction with Darcy's law. Each node (or cell) of the model includes a source/sink term, representing contaminants released or absorbed over time. The source/sink term may include equilibrium relations for volatilization/dissolution, sorption/desorption, and degradation. Vapor phase concentrations are calculated using mass balance relations in conjunction with the advection-dispersion equation. If high flow velocities are anticipated, dispersion may be neglected due to the predominance of advective transport.

Table C-1

Summary of Pressure Distribution, Airflow, and Vapor Transport Models for PCs

Model Name	Model Type and Use	Developer and Availability	Computer Requirements	Input Parameters	Output Parameters	Ease of Use
AIRFLOW/ SVE	2-D finite element radial symmetric airflow	Scientific Software Group Phone (703) 620-9214	IBM PC 386/486 with minimum of 4Mb RAM, EGA or VGA display, and a math coprocessor. A mouse is recommended.	Permeability, initial pressures, gas characteristics, temperature	Soil pressure distribution, total system flow	Easy
AIR2D, AIR3D	2-D and 3-D analytical radial-symmetric airflow	U.S. Geological Survey 810 Bear Tavern Road, Suite 206 West Trenton, NJ 08628 Phone: (609)-771-3901	IBM PC/AT compatible, 512K RAM	Permeability test data, initial pressures, flow rates	Permeability, pressure distribution and flow	Easy
BIOSLURP	2-D multiphase hydrocarbon vacuum enhanced recovery & transport model	Draper Aden Environmental Modeling, Inc. 2206 S. Main St. Blacksburg, VA 24060 (540) 961-DAEM	Windows 3.x/Windows 95/Windows NT and 8 MB RAM	Hydraulic properties, dispersivities, diffusion coefficients, biodegradation parameters, distribution coefficients, transfer rates.	Pressure, fluid saturation, velocity, pumping/injection rates, concentrations, and mass.	Moderate
BioSVE	Screening model to simulate vacuum enhanced recovery and biodegradation.	Draper Aden Environmental Modeling, Inc. 2206 S. Main St. Blacksburg, VA 24060 (540) 961-DAEM	Windows 3.x/Windows 95/Windows NT and 4 MB RAM	Air pumping rate, mass, bioefficiency, volume of contaminated soil, free product recovery parameters, and species-specific properties.	Mass of species in various phases and species well gas concentration vs. time.	Moderate
Hyper-Ventilate	Screening	Developed by: USEPA and Shell Oil Company Available through NTIS: 703/487-4650 Order #PB-93-502664/AS	HyperVentilate v2.0 for Microsoft Windows requires 386 or higher processor, 4 MB RAM minimum, and VGA or 8514. The software requirements are DOS 3.1 or higher, or Microsoft Windows 3.1 or higher.	Permeability, porosity, initial pressures, topography, boiling point data on spill components, and desired remediation time	Estimates of flow rates; removal rates; residual concentrations, no. of wells required	Easy
MAGNAS	2-D and 3-D finite element transport of water, NAPL, and air through porous media. Simulate flow of air as a fully active phase.	HydroGeologic, Inc. 1165 Hernadon Parkway, Suite 900, Hernadon, VA 22079 703/478-5186	IBM PC/AT compatible. Code documentation and user's manual is available. Written in FORTRAN 77.	Heterogeneous and anisotropic media properties, capillary pressures and permeability.	Breakthrough curves of concentration vs. time, flow and transport mass balances.	Difficult

Table C-1
(Concluded)

Model Name	Model Type and Use	Developer and Availability	Computer Requirements	Input Parameters	Output Parameters	Ease of Use
MODAIR	2-D or 3-D finite difference predictions of airflow in unsaturated zone.	Scientific Software Group Phone (703) 620-9214	PC 386/486 with 2 MB RAM. Requires SURFER or other graphics package for graphical output.	Unsaturated zone permeability, pressure conditions, vacuum rates.	Airflow distributions, pressures, velocities.	Moderate
MOD-FLOW	3-D finite difference groundwater flow (converted for air flow calculations)	U.S. Geological Survey 431 National Center Reston, VA 20192	IBM PC/AT compatible, DOS 3.3 or higher, math coprocessor, graphics monitor	Vapor conductivity, initial pressures	Soil pressure distribution; total system flow	Difficult
MOFAT	2-D finite element multiphase flow and multicomponent transport of up to 5 species	Draper Aden Environmental Modeling, Inc. 2206 S. Main St. Blacksburg, VA 24060 (540) 961-DAEM	Windows 3.x/Windows 95/Windows NT and 8 MB RAM.	Hydraulic properties, fluid properties, dispersivity, concentrations, partition and mass transfer coefficients.	Pressure heads, saturations, and velocities, and concentrations.	Moderate
MOVER	2-D finite element multiphase areal flow with vacuum enhanced recovery model.	Draper Aden Environmental Modeling, Inc. 2206 S. Main St. Blacksburg, VA 24060 (540) 961-DAEM	Windows 3.x/Windows 95/Windows NT and 8 MB RAM.	Initial conditions, boundary conditions, soil hydraulic properties, hydraulic conductivity, and porosity.	Spatial distribution of fluid pressure, saturation, velocity, and pumping/injection rates.	Moderate
P3DAIR	2-D or 3-D simulation of air flow and transport of vapor in unsaturated soils using MODFLOW	Scientific Software Group Phone (703) 620-9214	PC 486/Pentium with 2 MB RAM. Requires SURFER or other graphics package for output graphics.	Air pressure solutions from MODAIR, chemical specific parameters.	Spatial distribution of vapor concentrations and component mass.	Difficult
TIMES	2-D finite element simulations of dissolved constituents in water, airflow, and NAPL.	TriHydro Corporation (307) 745-7474	Windows 96/Windows NT, 486 and higher, and 8MB RAM minimum	Hydrogeologic and fluid characteristics, constituent specific parameters, NAPL, pumping and vacuum rates.	Water heads, pressure distribution, constituent concentrations, and air velocities.	Easy
VENTING						

3 Jun 02

b. For multiphase flow and contaminant transport models, the air pressure distribution is calculated by simultaneous solution of air, water, and NAPL flow equations. The equations are usually solved in terms of air-water, air-NAPL, and NAPL-water capillary pressures. Fluid mass balance is maintained using capillary pressure-saturation relations, which are also used to specify air, water, and NAPL permeabilities at each node (or cell).

c. Fluid velocities are calculated using pressure (or head) distributions in conjunction with Darcy's law. Contaminant partitioning is specified by source/sink terms for each node, and contaminant concentrations are calculated using mass balance relations in conjunction with the advection-dispersion equation. Because of the complexity of multiphase flow models, simplifying assumptions are often used. Depending on the assumptions involved, some models may be more appropriate for NAPL or dissolved phase transport than vapor transport.

d. Care is advised when using coupled fluid flow and contaminant transport models. Most of these models are based upon the "local equilibrium assumption," which assumes that mass transfer to and from the air phase is instantaneous. In reality, mass transfer may be limited by diffusion or the kinetics of sorption/desorption and volatilization/dissolution. This tends to result in longer treatment times than model predictions. In addition, several model parameters may be difficult or impossible to measure (e.g., dispersivity, partitioning relations, and constitutive relations for multiphase flow). Although most of these parameters are treated as constants, some are known to vary as functions of both space and time (e.g., dispersivity). To evaluate the accuracy of model predictions, validation with field data (such as pumping tests), is recommended.

(1) Typical input parameters for coupled airflow and contaminant transport models include:

- Time stepping information.
- Bulk dry density of soil.
- Soil organic carbon content.
- Air-water, air-soil, and air-NAPL partition coefficients for each compound.
- Air permeability.
- Air-filled soil porosity.
- Volumetric moisture content of soils.
- Pumping rates at extraction points or injection points.
- Thickness and geometry of the vadose zone.
- Dynamic viscosity of vapor.
- Vapor temperature.

- Gas molar mass.
- Total mass of each compound in the system or rate of mass addition.
- Compound degradation rates.
- Air dispersion coefficients.
- Gas constant (R).
- Pressure boundary conditions.

(2) Additional parameters for multiphase flow and contaminant transport models include:

Capillary pressure-saturation relations.

Air-water, air-NAPL, and NAPL-water interfacial tensions.

Soil-water, NAPL-water, and NAPL-soil partition coefficients.

Water dispersion coefficients.

NAPL composition data.

(3) Output from fluid flow and contaminant transport models can include:

Air pressure distributions.

Flow rates at constant pressure boundaries.

Airflow velocities.

Airflow pathlines.

Mass removal rates of compounds in air.

Spatial and temporal distributions of chemical concentrations in air, soil, and water.